Advanced Crash Course in Supercomputing: Supercomputers, HPC Centers, and Batch Scripts

NCCS
National Center for Computational Sciences

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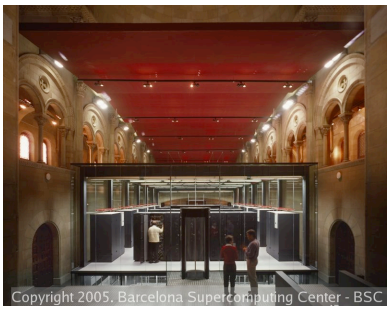
Outline

I. Supercomputers
II. Batch Scripts
III. Using Smoky



I. SUPERCOMPUTERS

Mare Nostrum, installed in Chapel Torre Girona, Barcelona Supercomputing Center. By courtesy of Barcelona Supercomputing Center -- http://www.bsc.es/

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I. Supercomputers

- Computer Architecture 101
- Life at an HPC Center

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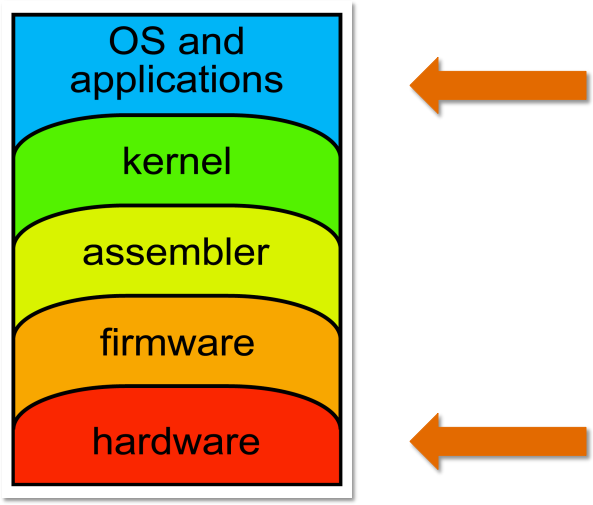
Computer Architecture 101



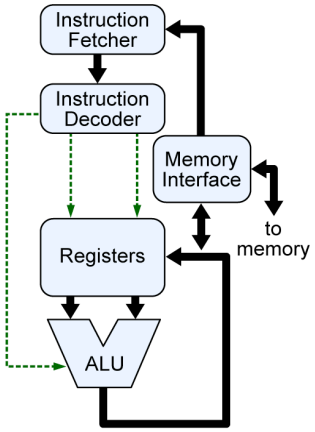
Source: http://en.wikipedia.org/wiki/Image:Computer_abstraction_layers.svg (author unknown)

Computer Architecture 101

- Processors
- Memory
  - Memory Hierarchy
  - TLB
- Interconnects
- Glossary

Computer Architecture 101: Processors

- CPU performs 4 basic operations:
  - Fetch
  - Decode
  - Execute
  - Writeback



Source: http://en.wikipedia.org/wiki/Image:CPU_block_diagram.svg

CPU Operations

- Fetch
  - Retrieve instruction from program memory
  - Location in memory tracked by program counter (PC)
  - Instruction retrieval sped up by caching and pipelining
- Decode
  - Interpret instruction by breaking into meaningful parts, e.g., opcode, operands
- Execute
  - Connect to portions of CPU to perform operation, e.g., connect to arithmetic logic unit (ALU) to perform addition
- Writeback
  - Write result of execution to memory

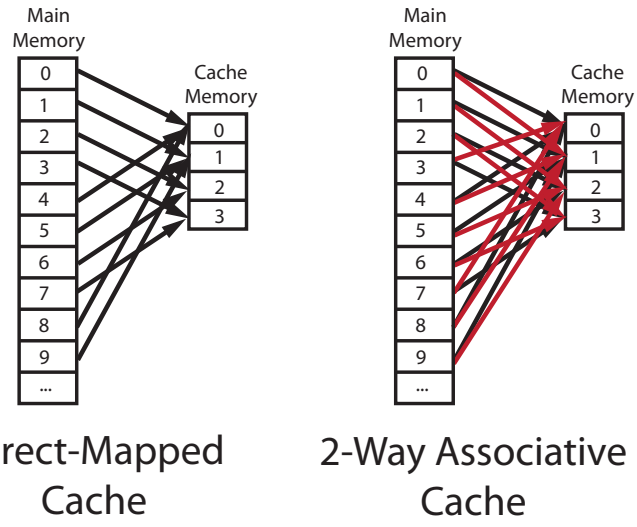
Computer Architecture 101: Memory

- Hierarchy of memory
  - Fast-access memory: small (expensive)
  - Slower-access memory: large (less expensive)
- Cache: fast-access memory where frequently used data stored
  - Reduces average access time
  - Works because typically, applications have locality of reference
  - Cache in XT4/5 also hierarchical
- TLB: Translation lookaside buffer
  - Used by memory management hardware to improve speed of virtual address translation

Cache Associativity

- Where to look in cache memory for copy of main memory location?
  - Direct-Mapped/ 1-way Associative: only one location in cache for each main memory location
  - Fully Associative: can be stored anywhere in cache
  - 2-way Associative: two possible locations in cache
  - *N*-way Associative: *N* possible locations in cache
- Doubling associativity (1 → 2, 2 → 4) has same effect on hit rate as doubling cache size
- Increasing beyond 4 does not substantially improve hit rate; higher associativity done for other reasons

Cache Associativity: Illustration



Direct-Mapped Cache

2-Way Associative Cache

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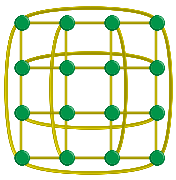
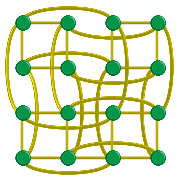
Computer Architecture 101: Interconnects

- Connect nodes of machine to one another
- Methods of interconnecting
  - Fiber + switches and routers
  - Directly connecting
- Topology
  - Torus
  - Hypercube
  - Butterfly
  - Tree



2-D Torus



Hypercube

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Computer Architecture 101: Glossary

- *SSE (Streaming SIMD Extensions):* instruction set extension to x86 architecture, allowing CPU to work on multiple instructions in single clock cycle
- *DDR2 (Double Data Rate 2):* synchronous dynamic random access memory, operates twice as fast as DDR1
  - DDR2-*xyz*: performs *xyz* million data transfers/second
- *Dcache:* cache devoted to data storage
- *Icache:* cache devoted to instruction storage
- *STREAM:* data flow

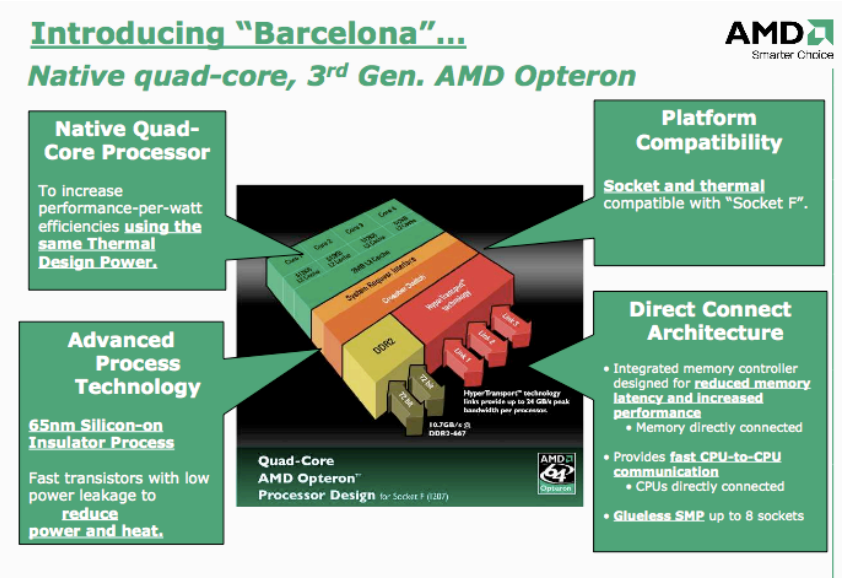
NCCS Facts and Figures

	Jaguar	Jaguarpf	Eugene
Compute Nodes	7832	18,772	2048
Processor	2.1 GHz AMD Opteron Quad Core	2.3 GHz AMD Opteron Dual Quad-Core	850MHz IBM quad core 450d PowerPC
Memory	2 GB/core DDR2-667/ DDR2-800	2 GB/core DDR2-800	2 GB/node
Network	Cray SeaStar 2	Cray SeaStar 2	3-D torus, 5.1 Gb/s
Peak	263 TF	1.3 PF	27 TF

XT4/5 Architecture

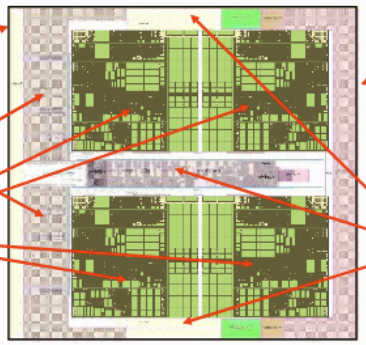
- Hardware
  - Processors
  - Memory
    - Memory Hierarchy
    - TLB
  - System architecture
  - Interconnects
- Software
  - Operating System Integration
  - CNL vs Linux

Quad-Core Architecture



AMD's Next Generation Processor Technology

AMD Smarter Choice



- 32B instruction fetch
- Improved branch prediction
- Out-of-order load execution
- Up to 4 DP FLOPS/cycle
- Dual 128-bit SSE dataflow
- Dual 128-bit loads per cycle
- Instruction Extensions
- Power Management Extensions

- Enhanced HyperTransport™ links
- Enhanced crossbar
- DDR2 with migration path to DDR3
- Enhanced power management and RAS

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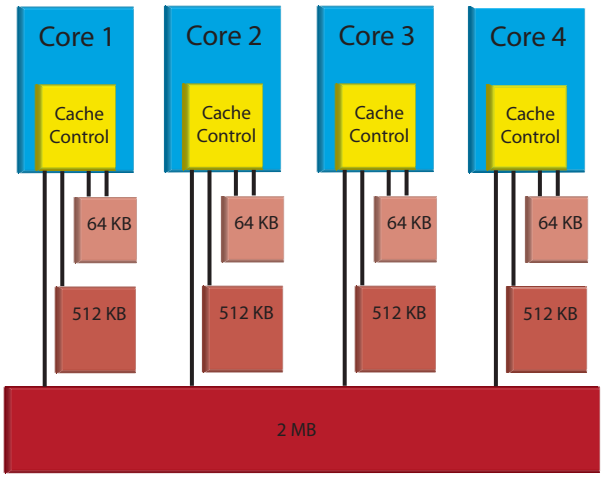
Quad Core Cache Hierarchy



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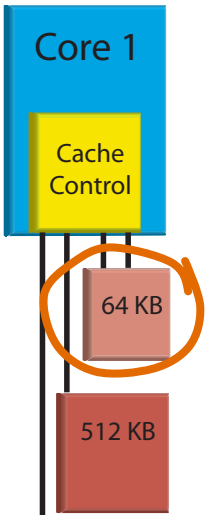
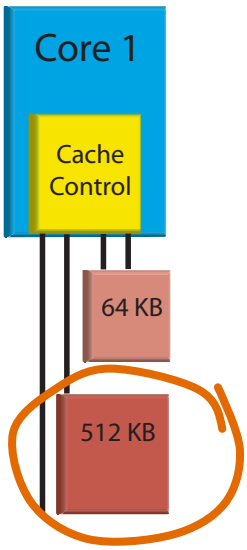
L1 Cache

- Dedicated
- 2-way associativity
- 8 banks
- 2 x 128-bit loads/cycle



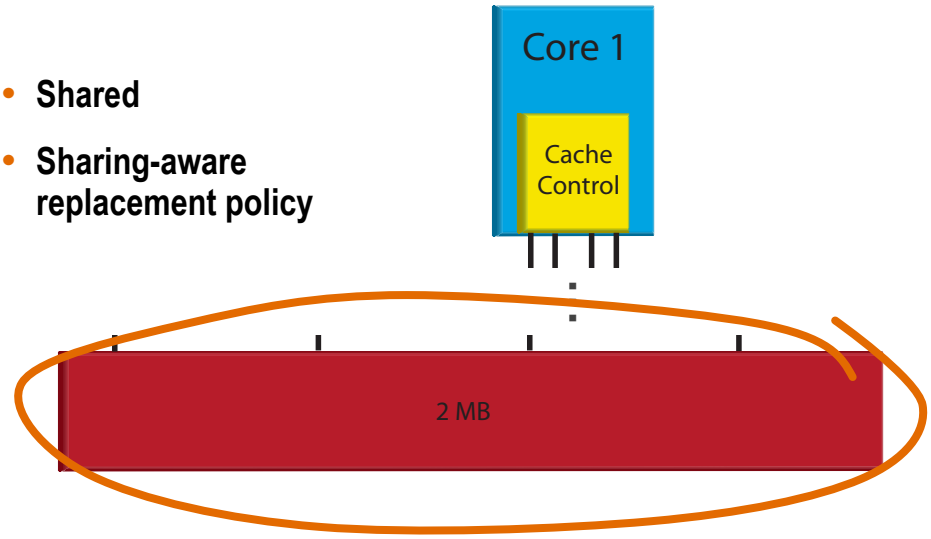
L2 Cache

- Dedicated
- 16-way associativity

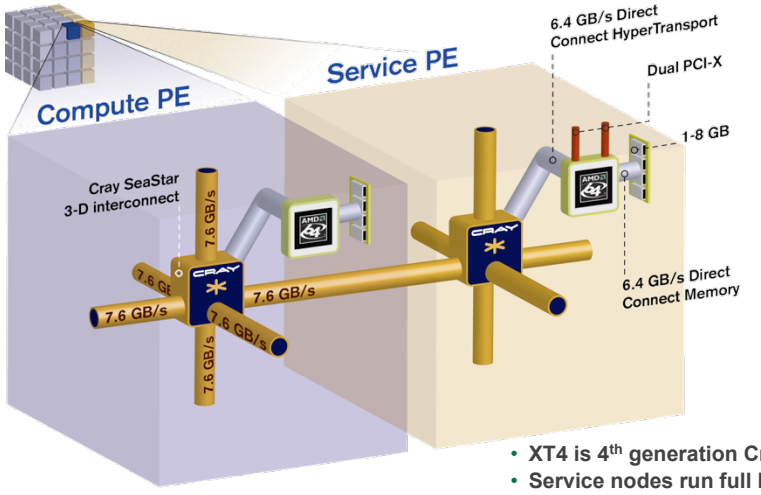


L3 Cache

- Shared
- Sharing-aware replacement policy



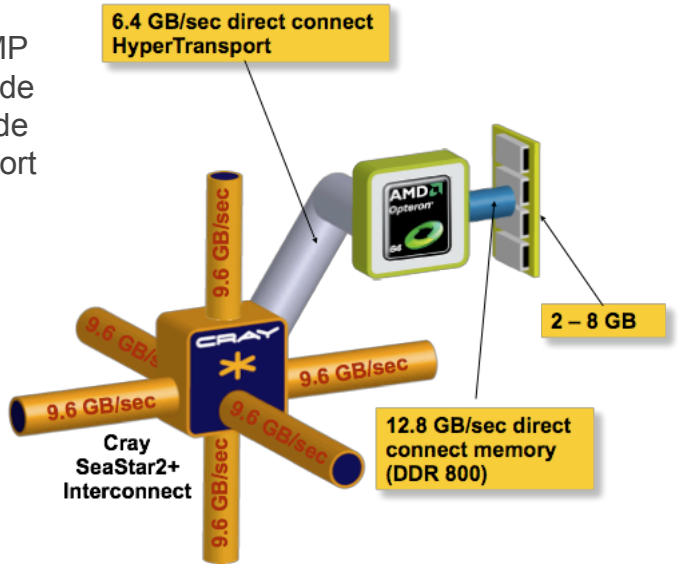
Cray XT4 Architecture



- XT4 is 4th generation Cray MPP
- Service nodes run full Linux
- Compute nodes run Compute Node Linux (CNL)

Cray XT4 Architecture

- 2- or 4-way SMP
- > 35 Gflops/node
- Up to 8 GB/node
- OpenMP Support within Socket



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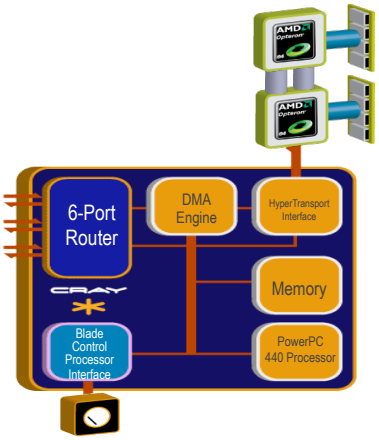
Cray SeaStar2 Architecture

- **Router connects to 6 neighbors in 3-D torus**
  - **Peak bidirectional BW 7.6 GB/s; sustained 6 GB/s**
  - **Reliable link protocol with error correction and retransmission**
- **Communications Engine: DMA Engine + PPC 440**
  - **Together, perform messaging tasks so AMD processor can focus on computing**
- **DMA Engine and OS together minimize latency with path directly from app to communication hardware (without traps and interrupts)**



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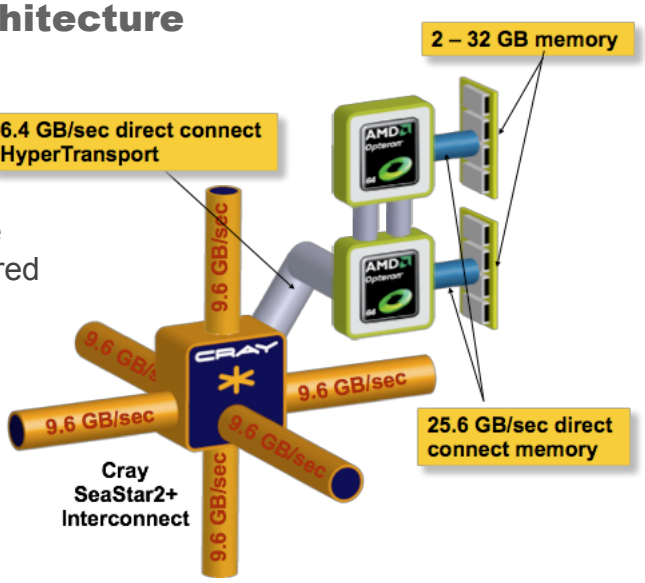
Cray XT5 Architecture

- 8-way SMP
- > 70 Gflops/node
- Up to 32 GB shared memory/node
- OpenMP support



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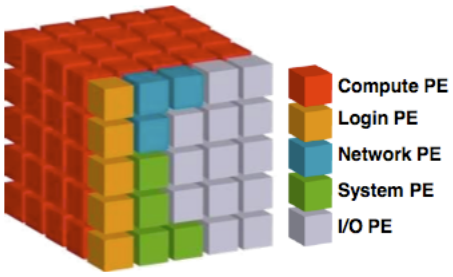
Software Architecture



Service Partition
Specialized Linux nodes

- CNL microkernel on compute nodes
- Full-featured Linux on service nodes
- Software architecture eliminates jitter and enables reproducible runtimes
- Even large machines can reboot in < 30 mins, including filesystem

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Software Architecture

- *Compute PE (processing element):* used for computation only; users cannot directly access compute nodes
- *Service PEs:* run full Linux
  - *Login:* users access these nodes to develop code and submit jobs, function like normal Linux box
  - *Network:* provide high-speed connectivity with other systems
  - *System:* run global system services such as system database
  - *I/O:* provide connectivity to GPFS (global parallel file system)

CNL vs Linux

- CNL (Compute-Node Linux) contains subset of Linux features
- Minimizes system overhead because little between application and bare hardware

Life at an HPC Center

- Work
- People
- Careers

Life at an HPC Center: Work

- Vendor
  - Install/maintain machine at center
  - Support customers
  - Support/improve current software environment
  - Develop next architecture, software
  - Market products
- Center
  - Maintain system
  - Develop/maintain power/ cooling infrastructure
  - Support users
  - Maintain system software
  - Develop next architecture/software
  - Outreach to public, Congress, funding agencies
  - Perform original research

Life at an HPC Center: People

- Vendor
  - Computer Architects
  - Software Developers
  - Mathematicians and Science Experts
  - Electrical Engineers
  - Electricians
  - Installers
  - Customer support liaisons
- Center
  - System administrators
  - Network engineers
  - System security experts
  - User support specialists
  - Education specialists
  - Science writers
  - Web Developers
  - Application Scientists
  - Computer Architects
  - Electrical, Civil, Mechanical Engineers
  - Electricians
  - Project Managers
  - Finance/Accounting managers

Life at an HPC Center: Careers

- Five groups in NCCS
  - User Assistance and Outreach
    - Helping users access machines, technical support, education, publications
  - Scientific Computing
    - Science experts helping users to take advantage of NCCS resources
  - Technology Integration
    - Develop infrastructure that supports NCCS systems and keep it ahead of technology curve
  - High Performance Computing
    - Keep systems up and running
  - Cray Center for Excellence
    - System expertise to facilitate breakthrough science on Cray architectures

Life at an HPC Center: Careers

- NCCS is good place to work
  - Good pay, benefits
  - Smart and nice colleagues
  - Can work your way up

Resources: Computer Architecture 101

- Wikipedia articles on computer architecture:
  http://en.wikipedia.org/wiki/Computer_architecture ,
  http://en.wikipedia.org/wiki/CPU ,
  http://en.wikipedia.org/wiki/CPU_cache ,
  http://en.wikipedia.org/wiki/DDR2_SDRAM ,
  http://en.wikipedia.org/wiki/Microarchitecture ,
  http://en.wikipedia.org/wiki/SSE2 ,
  http://en.wikipedia.org/wiki/Streaming_SIMD_Extensions
- Heath, Michael T. (2007) *Notes for CS 554, Parallel Numerical Algorithms*,
  http://www.cse.uiuc.edu/courses/cs554/notes/index.html

Resources: Cray XT4 Architecture

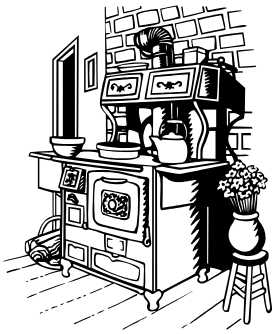
- Local machines
  - Jaguar: http://www.nccs.gov/computing-resources/jaguar/
  - Eugene: http://www.nccs.gov/computing-resources/eugene/
  - Jaguarpf: http://www.nccs.gov/jaguar/
- AMD architecture
  - Waldecker, Brian (2008) *Quad Core AMD Opteron Processor Overview*, available at http://www.nccs.gov/wp-content/uploads/2008/04/amd_craywkshp_apr2008.pdf
  - Larkin, Jeff (2008) *Optimizations for the AMD Core*, available at http://www.nccs.gov/wp-content/uploads/2008/04/optimization1.pdf
- XT4 Architecture
  - Hartman-Baker, Rebecca (2008) *XT4 Architecture and Software*, available at http://www.nccs.gov/wp-content/training/2008_users_meeting/4-17-08/using-xt44-17-08.pdf

II. BATCH SCRIPTS

Soft Batch Cookies. From http://www.kelloggconvenience.com/Resources/Soft_Batch-Home-PBpouch.jpg

II. Batch Scripts

- Batch system and Scheduling
- Concepts
- Useful commands
- Further help



Batch System and Scheduling

- Supercomputer: powerful computer consisting of many interlinked CPUs
- Users competing for computational resources
- How to launch and schedule jobs fairly?
- Job can run without user presence
- Must not allow one user to hog resources

Batch System

- Batch system accepts input jobs into queue and launches them when resources available
- Many machines use batch system PBS (*P*ortable *B*atch *S*ystem)
- PBS developed for NASA in 1990s

Scheduler

- Scheduler decides when jobs can be run based on scheduling policies, e.g. user priority, length of job, number of nodes requested, length of time in queue
- Many machines use Maui Scheduler
- Maui Scheduler extensively developed, supported by large segment of computation community including U.S. Dept. of Energy, NCSA

(source: www.the-hawaii-vacation-guide.com)

Concepts

- Limits for walltime and number of processors, so if request exceeds limits, job automatically rejected
- Scheduler rules complicated, but generally, "smaller" jobs run first
- Size of job is function of number of processors and estimated time
- You provide info about number of processors you want and estimate of time job will run

Concepts

- Strategies:
  - Like inverse of "The Price Is Right," give lowest estimate possible, without going under true time needed (always good strategy)
  - Use fewer processors if possible (not always good strategy)
- If you reach end of estimated time, PBS will terminate your job!
- Write script that tells PBS what to do when job is launched

Concepts

- Shell Script format:
  - First, a line invoking the scripting language:

    `#!/bin/csh`
  - Next, embedded PBS commands, e.g.
    `#PBS -l walltime=00:10:00,nodes=2:ppn=2`
    `#PBS -q workq`
    (the shell script interprets these as comments, but PBS understands they are PBS commands)
  - Then, environment variable initialization, e.g.
    `setenv MYMAINDIR /home/hqi/hello` (sets variable `MYMAINDIR` to `/home/hqi/hello`)
    `setenv PROG $MYMAINDIR/prog` (sets `PROG` to `/home/hqi/hello/prog`)

Concepts

- Shell script format (continued):
  - Then, shell script and regular Linux commands, e.g.

    `if (-e $OUTF) mv $OUTF $OUTF.old`

    (meaning that if file called `$OUTF` exists, rename it to `$OUTF.old`)
  - Finally, run job:

    `mpirun -np $NP $PROG < $INFILE > $OUTF`
- To launch job:
  - Make script executable*: `chmod u+x myscript`
  - `qsub myscript`

*Not necessary on some systems

Useful Commands (PBS)

- `#PBS -l walltime=hh:mm:ss,nodes=n:ppn=p` This tells PBS how much walltime you request (where `hh:mm:ss` replaced by appropriate number of hours, minutes, and seconds), how many *dual processor* nodes you want (replace `n` with appropriate number), *and how many processors per node (1, 2, 3, or 4)*
- `#PBS -q workq` Which queue to use (in this case, queue called workq)
- `#PBS -V` Export all environment variables to batch job (good practice to do this)
- `#PBS -m be` Sends you e-mail at beginning and end of job

Useful Commands (Shell Scripting)

- `set echo` Print out commands as they are executed (useful for debugging script)
- `setenv A B` or `export A=B` Sets environment variable `A` to `B`
- `$A` value of `A`
- `mpirun -np $NP $PROG < $INPUT`
  `mpirun` (sometimes `mpiexec`, or on proprietary systems, `aprun`, `poe`, etc.) is executable that launches parallel jobs on multiple processors; `-np` is flag indicating number of processors used in run

  *NOTE: some implementations do not require input redirection (<)

Further Help

- NCSA Cobalt Documentation: Running Jobs http://www.ncsa.uiuc.edu/UserInfo/Resources/Hardware/SGIAltix/Doc/Jobs.html
- The C Shell tutorial http://www.eng.hawaii.edu/Tutor/csh.html
- DuBois, Paul. *Using csh & tcsh,* O'Reilly & Associates, 1995.
- Newham, Cameron and Bill Rosenblatt. *Learning the bash Shell,* O'Reilly & Associates, 1998.

Bibliography/Resources

- About OpenPBS http://www.openpbs.org/about.html
- Maui Scheduler http://www.supercluster.org/maui/

III. USING SMOKY

Sunset from Clingmans Dome, Great Smoky Mountains National Park, photo available at http://www.nps.gov/grsm/photosmultimedia/index.htm

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III. Using Smoky

- About Smoky
- Logging In
- Compiling
- Software Environment
- Running Jobs

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About Smoky

- Development cluster, comparable to larger NCCS machines
- Used for application development
- 80 node Linux cluster
- Each node consists of four quad-core 2.0 GHz AMD Opteron processors, with 32 GB memory (2GB/core)
- Gigabit ethernet network with infiniband interconnect

Logging in to Smoky

- Use ssh to connect

  `ssh` *`username`*`@smoky.ccs.ornl.gov`

- Authentication using one-time passwords from RSA SecurID key fob
- X11 Tunneling: use `-X` (or on a Mac, `-Y`) option with ssh

Compiling on Smoky

- Three compiler suites available on smoky:
  - PGI (default)
  - Pathscale
  - GCC
- MPI compilers (wrappers to compiler independent of programming environment)
  - `mpicc` (C compiler)
  - `mpiCC` (C++ compiler)
  - `mpif77` (Fortran 77 compiler)
  - `mpif90` (Fortran 90 compiler)

Software Environment on Smoky

- Suppose I need to use GNU C++ compiler to compile my code
- Suppose I also want to link with the PETSc library
- On most systems, would need to change paths in makefiles each time I port to new system
- Would need to make sure to point to GNU compiler and proper build of PETSc
- What happens if I discover that I need a different compiler? Go back and change everything again

Software Environment on Smoky

- Modules allow dynamic modification of user environment with modulefiles
- Can switch from PGI to GNU and back again with simple command
- Can load proper version of PETSc automatically, based on compiler loaded

Software Environment on Smoky: Modules

- Software is loaded or swapped using modules
- Allows software, libraries, paths, etc. to be cleanly entered into and removed from your programming environment
- Conflicts are detected and loads that would cause conflicts are not allowed

Software Environment on Smoky: Modules

Command	Definition	Example
`module load my_module`	Loads module *my_module*	`module load petsc`
`module swap first_module second_module`	Replaces *first_module* with *second_module*	`module swap PE-pgi PE-gnu`
`module help`	Lists available commands and usage	
`module list`	Lists all modules currently loaded	
`module avail [name]`	Lists all modules [beginning with *name*]	`module avail gcc`

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Running Jobs on Smoky

- **Login node: node you log in to**
  - **Edit files**
  - **Code compilation**
  - **Data backup**
  - **Job submission**
- **Compute nodes**
  - **Where jobs run**
  - **Access managed by PBS**
  - **Scheduling by Moab**

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Nice Job Script for Smoky

```
#PBS -V
#PBS -j oe
#PBS -A STF006
#PBS -N loadbal
#PBS -l walltime=00:10:00,nodes=1:ppn=16
export CURRDIR="/ccs/home/hqi/hello"
export SCRDIR="/tmp/work/hqi"
export EXEC="hello"
export INPUT_FILE="hello_input"
cp $CURRDIR/$EXEC $SCRDIR
cp $CURRDIR/$INPUT_FILE $SCRDIR
cd $SCRDIR
date
mpirun -n 16 ./$EXEC < $INPUT_FILE
date
```


Resources/Bibliography

- **Smoky webpage**
  http://www.nccs.gov/computing-resources/smoky/
- **NCCS Modules webpage**
  http://www.nccs.gov/user-support/general-support/modules/